

STN Columbus

***** Welcome to STN International *****

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 NEWS 3 JUL 28 EPFULL enhanced with additional legal status
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 NEWS 5 JUL 28 STN Viewer performance improved
 NEWS 6 AUG 01 INPADOCDB and INPAFAMDB coverage enhanced
 NEWS 7 AUG 13 CA/Caplus enhanced with printed Chemical Abstracts
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 NEWS 15 SEP 29 EMBASE and EMBAL enhanced with new search and
 display fields
 NEWS 16 SEP 30 CAS patent coverage enhanced to include exemplified
 prophetic substances identified in new Japanese-
 language patents
 NEWS 17 OCT 07 EPFULL enhanced with full implementation of EPC2000
 NEWS 18 OCT 07 Multiple databases enhanced for more flexible patent
 number searching
 NEWS 19 OCT 22 Current-awareness alert (SDI) setup and editing
 enhanced
 NEWS 20 OCT 22 WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT
 Applications
 NEWS 21 OCT 24 CHEMLIST enhanced with intermediate list of
 pre-registered REACH substances
 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
 AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.
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FILE 'HOME' ENTERED AT 00:36:50 ON 19 NOV 2008

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 00:37:14 ON 19 NOV 2008
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STRUCTURE FILE UPDATES: 17 NOV 2008 HIGHEST RN 1073055-74-9
DICTIONARY FILE UPDATES: 17 NOV 2008 HIGHEST RN 1073055-74-9

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e abacavir/cn

E1 1 ABACA/CN
E2 1 ABACA MANILA HEMP/CN
E3 1 --> ABACAVIR/CN
E4 1 ABACAVIR 5'-MONOPHOSPHATE DEAMINASE/CN
E5 1 ABACAVIR MONOPHOSPHATE DEAMINASE/CN
E6 1 ABACAVIR SUCCINATE/CN
E7 1 ABACAVIR SULFATE/CN
E8 1 ABACAVIR SULFATE-LAMIVUDINE MIXT./CN
E9 1 ABACAVIR-EPIVIR MIXT./CN
E10 1 ABACIL/CN
E11 1 ABACIN/CN
E12 1 ABACOPTERIN A/CN

=> s e3

L1 1 ABACAVIR/CN

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

RN 136470-78-5 REGISTRY

ED Entered STN: 04 Oct 1991

CN 2-Cyclopentene-1-methanol, 4-[2-amino-6-(cyclopropylamino)-9H-purin-9-yl]-, (1S,4R)- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Cyclopentene-1-methanol, 4-[2-amino-6-(cyclopropylamino)-9H-purin-9-yl]-, (1S-cis)-

OTHER NAMES:

CN 1592089

CN **Abacavir**

CN Ziagen

FS STEREOSEARCH

MF C14 H18 N6 O

CI COM

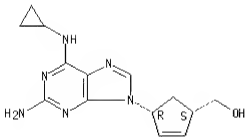
SR CA

LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CBNE, CHEMCATS, CIN, CSCHEM, DDFU, DRUGU, EMBASE, IMSDRUGNEWS, IMSPATENTS, IMSPRODUCT, IMSRESEARCH, IPA, MRCK*, PATDPASPC, PHAR, PIRA, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL

(*File contains numerically searchable property data)

Other Sources: WHO

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1298 REFERENCES IN FILE CA (1907 TO DATE)
 16 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 1305 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file merck
 COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.61	7.82

FULL ESTIMATED COST

FILE 'MRCK' ENTERED AT 00:37:44 ON 19 NOV 2008

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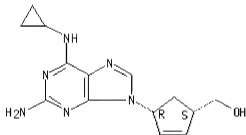
=> s ll

L2 1 L1

=> d all

L2 ANSWER 1 OF 1 MRCK COPYRIGHT (C) 2008 Merck and Co., Inc.,
 Whitehouse Station, New Jersey, USA. All rights reserved. on SIN
 MERCK Number (MNO): 1400001
 CAS Registry No. (RN): **136470-78-5**
 MERCK Index Name (MIN): Abacavir
 CA Index Name (CN): (1S,4R)-4-[2-Amino-6-(cyclopropylamino)-9H-purin-9-yl]-
 2-cyclopentene-1-methanol
 Synonym(s) (CN): (-)-cis-4-[2-amino-6-(cyclopropylamino)-9H-purin-9-yl]-
 2-cyclopentene-1-methanol
 Drug Code(s) (CN): 1592U89
 File Segment. (FS): Active Monographs
 Molecular Form. (MF): C14 H18 N6 O
 Wgt Composition (COMP): C 58.73%, H 6.34%, N 29.35%, O 5.59%.
 Molecular Weight (MW): 286.33
 References (RE): Nucleoside reverse transcriptase inhibitor (NRTI).
 Prep: S. M. Daluge, EP 349242 (1990 to Wellcome Found.); idem, US
 5034394 (1991 to Burroughs Wellcome). Asymmetric synthesis: M. T.
 Crimmins, B. W. King, J. Org. Chem. 61, 4192 (1996). Pharmacology and
 biological profile: S. M. Daluge et al., Antimicrob. Agents Chemother.
 41, 1082 (1997). Review of antiviral activity and clinical evaluations:
 R. H. Foster, D. Faulds, Drugs 55, 729-736 (1998). Clinical trial of
 triple nucleoside regimen in HIV patients: S. Staszewski et al., J. Am.
 Med. Assoc. 285, 1155 (2001).

Absolute stereochemistry. Rotation (-).



Melting Point (MP):

Value
MP
deg C

165

Optical Rotatory Power (ORP):

Value	Temp.	Spectral	Note
ORP	ORP.T	Line	
deg	deg C	ORP.SL	
-59.7	20	D	
-127.8	20	436	
-218.1	20	365	(c = 0.15 in methanol)

UV Spectrum (UVS):

Maximum	Note
Peak Pos.	
UVS.PP	
nm	
296	(pH 1) (ε 14000, 10700)
255	

Other Properties (OCP):

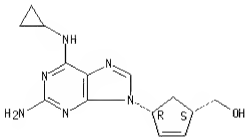
White solid foam from acetonitrile, mp 165°. . uv max (pH 1): 296
 , 255 nm (ε 14000, 10700) ; uv max (pH 7): 284 , 259 nm
 (ε 15900, 9200) ; uv max (pH 13): 284 , 259 nm (ε 15800,
 9100) . [α]_D20 -59.7° ; [α]_D3620 -127.8° ;
 [α]_D36520 -218.1° (c = 0.15 in methanol) . Log P
 (1-octanol/0.1M sodium phosphate): 1.22 ±0.03 (pH 7.4). pKa 5.01.
 Soly in water (25°): >80 mM (pH 7).

-- DERIVATIVE --

(1): Sulfate
 CAS Registry No. (RN.DRV): 188062-50-2
 Trade Name(s) (CN.DRV): Ziagen (GlaxoSmithKline plc; GSK)
 Molecular Form. (MF.DRV): (C₁₄ H₁₈ N₆ O)₂ . H₂ O₄ S
 Wgt Composition (COMP.DRV): C 50.14%, H 5.71%, N 25.06%, O 14.31%, S 4.78%.
 Molecular Weight (MW.DRV): 670.74

CM 1

Absolute stereochemistry. Rotation (-).



CM 2



Therapeutic Codes (THER):
 Antiretroviral.
 Referenced Patent (RPN):
 EP349242; US5034394

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-> file reg
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                               ENTRY      SESSION
FULL ESTIMATED COST          4.11      11.93
  
```

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 DICTIONARY FILE UPDATES: 17 NOV 2008 HIGHEST RN 1073055-74-9

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 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

```

-> e brivudine/cn
E1      1      BRIVOLIIDE J/CN
E2      1      BRIVUDIN/CN
E3      1 --> BRIVUDINE/CN
E4      1      BRIX (HUMAN CLONE MGC:45062 IMAGE:5107954)/CN
E5      1      BRIX (HUMAN CLONE MGC:4924 IMAGE:3462041 GENE BRIX)/CN
E6      1      BRIX (XENOPUS LAEVIS GENE BRIX)/CN
E7      1      BRIX DOMAIN CONTAINING 1 (HUMAN CLONE MGC:21067 IMAGE:474552
          4 GENE BXDCL1)/CN
E8      1      BRIX DOMAIN CONTAINING 1 (HUMAN CLONE MGC:21067 IMAGE:474552
          4)/CN
E9      1      BRIX DOMAIN CONTAINING 1 (MOUSE STRAIN CZECH II CLONE MGC:35
  
```

E10 1 797 IMAGE:4009314)/CN
BRIX DOMAIN CONTAINING-LIKE PROTEIN (LEISHMANIA MAJOR STRAIN
FRIEDLIN)/CN
E11 1 BRIX DOMAIN PROTEIN (SULFOLOBUS ACIDOCALDARIUS STRAIN DSM 63
9)/CN
E12 1 BRIX-DOMAIN RIBOSOMAL BIOGENESIS PROTEIN (METHANOBREVIBACTER
SMITHII STRAIN ATCC 35061)/CN

=> s e3

L3 1 BRIVUDINE/CN

=> d

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

RN 69304-47-8 REGISTRY

ED Entered STN: 16 Nov 1984

CN Uridine, 5-[(1E)-2-bromoethenyl]-2'-deoxy- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Uridine, 5-(2-bromoethenyl)-2'-deoxy-, (E)-

OTHER NAMES:

CN (E)-5-(2-Bromovinyl)-2'-deoxyuridine

CN (E)-5-(2-Bromovinyl)deoxyuridine

CN (E)-5-O-(2-bromoethenyl)-2'-deoxyuridine

CN 5-[(E)-2-Bromoethenyl]-2'-deoxyuridine

CN Brivudin

CN **Brivudine**

CN Bromovinyldeoxyuridine

CN BVDU

CN Helpin

FS STEREOSEARCH

DR 102040-00-6, 155203-57-9, 286419-83-8

MF C11 H13 Br N2 O5

CI COM

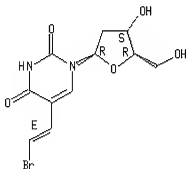
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS,
BIOTECHNO, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CIN, CSCHEM,
DDFU, DRUGU, EMBASE, IMSDRUGNEWS, IMPATENTS, IMSPRODUCT, IMSRESEARCH,
IPA, MEDLINE, PATDPASPC, PHAR, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE,
TOXCENTER, USAN, USPAT2, USPATFULL, VETU

(*File contains numerically searchable property data)

Other Sources: WHO

Absolute stereochemistry.

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

576 REFERENCES IN FILE CA (1907 TO DATE)

27 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

579 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

7.61

19.54

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DICTIONARY FILE UPDATES: 17 NOV 2008 HIGHEST RN 1073055-74-9

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on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

```
=> e cidofovir/cn
E1      1      CIDIROL/CN
E2      1      CIDOCETINE/CN
E3      1 -->  CIDOFOVIR/CN
E4      1      CIDOFOVIR DIPHOSPHATE/CN
E5      1      CIDOFOVIR HYDRATE/CN
E6      1      CIDOMYCIN/CN
E7      1      CIDOPHAGE/CN
E8      1      CIDOPHYLINE/CN
E9      1      CIDOTEN/CN
E10     1      CIDOVIR/CN
E11     1      CIDOXEPIN/CN
E12     1      CIDOXEPIN HYDROCHLORIDE/CN

=> s e3
L4      1      CIDOFOVIR/CN

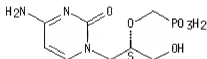
=> d

L4      ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN      113852-37-2  REGISTRY
ED      Entered STN:  16 Apr 1988
CN      Phosphonic acid, P-[[[(1S)-2-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-
(hydroxymethyl)ethoxy)methyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN      Phosphonic acid, [[[(1S)-2-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-
(hydroxymethyl)ethoxy)methyl]- (9CI)
CN      Phosphonic acid, [[2-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-
(hydroxymethyl)ethoxy)methyl]-, (S)-
OTHER NAMES:
CN      (S)-1-(3-hydroxy-2-phosphonomethoxypropyl)cytosine
CN      (S)-HPMPC
CN      1-(S)-1-(3-Hydroxy-2-phosphonylmethoxypropyl)cytosine
CN      1-[(S)-3-Hydroxy-2-(phosphonomethoxy)propyl]cytosine
CN      Cidofovir
CN      Cidovir
CN      GS 0504
CN      HPMPC
CN      Vistide
FS      STEREOSEARCH
MF      C8 H14 N3 O6 P
CI      COM
SR      CA
LC      STN Files:  ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS,
BIOTECHNO, CA, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST,
CIN, DDFU, DRUGU, EMBASE, HSDB*, IMSCOSEARCH, IMSDRUGNEWS, IMSPATENTS,
```

IMSPRODUCT, IMSRESEARCH, IPA, MEDLINE, MRCK*, MSDS-OHS, PATDPASPC, PHAR,
PROMT, PROUSDDR, PS, RTECS*, SCISEARCH, SYNTHLINE, TOXCENTER, USAN,
USPAT2, USPATFULL, VETU

(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

836 REFERENCES IN FILE CA (1907 TO DATE)
36 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
840 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file merck
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.61	27.15

FULL ESTIMATED COST

FILE 'MRCK' ENTERED AT 00:39:38 ON 19 NOV 2008

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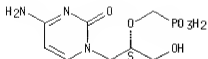
=> s l4

L5 1 L4

=> d all

L5 ANSWER 1 OF 1 MRCK COPYRIGHT (C) 2008 Merck and Co., Inc.,
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MERCK Number (MNO): 1402268
CAS Registry No. (RN): **113852-37-2**
MERCK Index Name (MIN): Cidofovir
CA Index Name (CN): [(1S)-2-(4-Amino-2-oxo-1(2H)-pyrimidinyl)-1-(hydroxymethyl)ethoxy)methyl]phosphonic acid
Synonym(s) (CN): (S)-1-[3-hydroxy-2-(phosphonylmethoxy)propyl]cytosine;
(S)-HPMPC
Drug Code(s) (CN): GS-504
Trade Name(s) (CN): Vistide (Gilead Sciences; Gilead)
File Segment. (FS): Active Monographs
Molecular Form. (MF): C8 H14 N3 O6 P
Wgt Composition (COMP): C 34.42%, H 5.05%, N 15.05%, O 34.38%, P 11.09%.
Molecular Weight (MW): 279.19
References (RE): DNA synthesis inhibitor. Prepn: A. Holy et al., EP 253412; eidem, US 5142051 (1988, 1992 both to Ceskoslov. Akad. Ved; Rega Inst.); and activity vs cytomegalovirus: R. Snoeck et al., Antimicrob. Agents Chemother. 32, 1839 (1988). Syntheses: J. J. Bronson et al., Nucleosides Nucleotides 9, 745 (1990); P. R. Brodfuehrer et al., Tetrahedron Lett. 35, 3243 (1994). Activity vs herpes simplex virus: G. Andrei et al., Eur. J. Clin. Microbiol. Infect. Dis. 11, 143 (1992). Review of pharmacology and clinical studies: M. J. M. Hitchcock et al., Antivir. Chem. Chemother. 7, 115-127 (1996). Review of clinical potential in poxvirus infections: E. De Clercq, Trends Pharmacol. Sci. 23, 456-458 (2002).

Absolute stereochemistry.



Melting Point (MP):

Value	Note
MP	
deg C	
=====	
260	(dec)

Optical Rotatory Power (ORP):

Value	Temp.	Spectral	Line	Note
ORP	ORP.T	ORP.SL		
deg	deg C			
=====				
-97.3	20	D		(c = 0.80 in water)

UV Spectrum (UVS):

Maximum	Note
Peak Pos.	
UVS.PP	
nm	
=====	
279	(pH 2) (ε 13000)

Other Properties (OCPP):

Fluffy white powder, mp 260° (dec) . [α]_{D20} -97.3°
 (c = 0.80 in water) . Monohydrate, uv max (pH 2): 279 nm (ε
 13000) .

Therapeutic Codes (THER):

Antiviral.

Referenced Patent (RPN):

EP253412; US5142051

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

2.79

29.94

STN INTERNATIONAL LOGOFF AT 00:40:13 ON 19 NOV 2008